

Statistical properties of the quantum anharmonic oscillator in one spatial dimension.

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1 Abstract

The random matrix ensembles (RME) of Hamiltonian matrices, e.g. Gaussian random matrix ensembles (GRME) and Ginibre random matrix ensembles (Ginibre RME), are applicable to following quantum statistical systems: nuclear systems, molecular systems, condensed phase systems, disordered systems, and two-dimensional electron systems (Wigner-Dyson electrostatic analogy). A family of quantum anharmonic oscillators in one spatial dimension is studied and the numerical investigation of their eigenenergies is presented. The statistical properties of the calculated eigenenergies are compared with the theoretical predictions inferred from the random matrix theory. Conclusions are derived.

2 Quantum harmonic oscillator in $D = 1$ spatial dimension.

Firstly: Let us consider the Hilbert space:

$$\mathcal{V}_1 = L^2(\mathbf{R}, \mathbf{C}, dx), \quad (1)$$

of the complex valued wave functions Ψ that are (modulus) square integrable on the set \mathbf{R} of the real numbers, and \mathbf{C} is the set of the complex numbers. The Hilbert space \mathcal{V}_1 is separable space, and its orthonormal basis \mathcal{B} is a set of Hermite's functions Ψ_r (Fok's functions, eigenfunctions of the dimensionless Hamiltonian operator $\hat{\mathcal{H}}$ of the quantum harmonic oscillator in $D = 1$ spatial dimension):

$$\Psi_r(x) = N_r H_r(x) \exp(-\frac{1}{2}x^2), N_r = [\sqrt{\pi} r! 2^r]^{-\frac{1}{2}}, r \in \mathbf{N}, \quad (2)$$

where \mathbf{N} is a set of natural numbers including zero, whereas:

$$H_r(x) = (-1)^r \exp(x^2) \frac{d^r}{dx^r} \exp(-x^2), \quad (3)$$

is r th Hermite's polynomial. We assume from now that all the operators are dimensionless (nondimensional). The dimensionless quantum operator \hat{x} of the x th component of the position vector (radius vector) acts on the Hermite's basis function as follows:

$$\hat{x}\Psi_r = \sqrt{\frac{r}{2}}\Psi_{r-1} + \sqrt{\frac{r+1}{2}}\Psi_{r+1}, \quad (4)$$

whereas the quantum operator \hat{p}_x of the x th component of linear momentum vector is given in the basis by the following formula:

$$\hat{p}_x\Psi_r = \frac{1}{i}\sqrt{\frac{r}{2}}\Psi_{r-1} - \frac{1}{i}\sqrt{\frac{r+1}{2}}\Psi_{r+1}. \quad (5)$$

Matrix elements $x_{l,r}$ and $(p_x)_{l,r}$ of these operators equal correspondingly:

$$x_{l,r} = \langle \Psi_l | \hat{x} \Psi_r \rangle = \sqrt{\frac{r}{2}}\delta_{l,r-1} + \sqrt{\frac{r+1}{2}}\delta_{l,r+1}, \quad (6)$$

and

$$(p_x)_{l,r} = \langle \Psi_l | \hat{p}_x \Psi_r \rangle = \frac{1}{i}\sqrt{\frac{r}{2}}\delta_{l,r-1} - \frac{1}{i}\sqrt{\frac{r+1}{2}}\delta_{l,r+1}, \quad (7)$$

where

$$\delta_{l,r} = \begin{cases} 1, & l = r \\ 0, & l \neq r \end{cases}, \quad (8)$$

is discrete Kronecker's delta (it is not continuous Dirac's delta). The quantum operator \hat{x}^2 of the square of the x th component of radius vector after acting on the basis function reads:

$$\hat{x}^2\Psi_r = \frac{1}{2}[\sqrt{r-1}\sqrt{r}\Psi_{r-2} + (2r+1)\Psi_r + \sqrt{r+1}\sqrt{r+2}\Psi_{r+2}], \quad (9)$$

and its matrix element $(x^2)_{l,r}$ is equal:

$$(x^2)_{l,r} = \frac{1}{2}[\sqrt{r-1}\sqrt{r}\delta_{l,r-2} + (2r+1)\delta_{l,r} + \sqrt{r+1}\sqrt{r+2}\delta_{l,r+2}], \quad (10)$$

whereas the quantum operator \hat{p}_x^2 of the square of the x th component of the linear momentum vector has the following representation in the basis:

$$\hat{p}_x^2\Psi_r = \frac{1}{2}[-\sqrt{r-1}\sqrt{r}\Psi_{r-2} + (2r+1)\Psi_r - \sqrt{r+1}\sqrt{r+2}\Psi_{r+2}], \quad (11)$$

and its matrix element $(p_x^2)_{l,r}$ is equal:

$$(p_x^2)_{l,r} = \frac{1}{2}[-\sqrt{r-1}\sqrt{r}\delta_{l,r-2} + (2r+1)\delta_{l,r} - \sqrt{r+1}\sqrt{r+2}\delta_{l,r+2}]. \quad (12)$$

Therefore, the dimensionless (nondimensional) quantum Hamiltonian operator $\hat{\mathcal{H}}$ reads:

$$\hat{\mathcal{H}} = \hat{p}_x^2 + \hat{x}^2, \quad (13)$$

acting on the basis function, it produces:

$$\hat{\mathcal{H}}\Psi_r = (2r+1)\Psi_r, \quad (14)$$

and its matrix element $\mathcal{H}_{l,r}$ is equal:

$$\mathcal{H}_{l,r} = (2r+1)\delta_{l,r}, \quad (15)$$

where

$$\epsilon_r = 2r+1, \quad (16)$$

is the r th eigenenergy of $\hat{\mathcal{H}}$. The eigenenergies are simply all odd natural numbers, and the quantum Hamiltonian is diagonal operator, and its matrix representation is diagonal $\infty \times \infty$ matrix. Note, that if one introduces the notion of nearest neighbour energy spacing (NNS):

$$s_r = \epsilon_{r+1} - \epsilon_r, r = 1, \dots, (N-1), N \geq 2, \quad (17)$$

then for the quantum harmonic oscillator it holds:

$$s_r = 2 = \text{const}, \quad (18)$$

so the eigenenergies are equidistant. Here N is the number of energies dealt with (it is also a dimension of truncated Hilbert space $\mathcal{V}_{1,N} \equiv \mathbf{C}^N$). The eigenfunctions of $\mathcal{V}_{1,N}$ are N -component constant complex vectors (analogs of spinors), and the operators acting on it are $N \times N$ deterministic complex-valued matrices. The probability distribution P_{N-1} of the spacings is discrete one point distribution for any finite value of $N, N \geq 2$:

$$P_{N-1}(s) = \frac{1}{N-1}\delta_{s,2}, \quad (19)$$

tending in the thermodynamical limit $N \rightarrow \infty$ to the singular Dirac's delta distribution:

$$P_\infty(s) = \delta(s-2). \quad (20)$$

Secondly, let us perform more difficult task consisting of calculating all the absolute moments:

$$(m_n)_{l,r} = m_n = (x^n)_{l,r} = \langle \Psi_l | \hat{x}^n | \Psi_r \rangle = \int_{-\infty}^{\infty} \Psi_l^*(x) x^n \Psi_r(x) dx, \quad (21)$$

of the position operator \hat{x} in the Hermite's (Fok's) basis \mathcal{B} . One can calculate the lower moments manually, e. g., using recurrence relations, matrix algebra, *etc.*, but it is tedious (even for $3 \leq n \leq 6$). If one wants to calculate *all* the moments then he must return to the beautiful XIX century mathematics methods and after some reasoning he obtains the exact formula:

$$\begin{aligned}
(m_n)_{l,r} &= m_n = (x^n)_{l,r} = \\
&= [1 - (-1)^{n+l+r}] \sum_{j=0}^{[l/2]} \sum_{k=0}^{[r/2]} [(-1)^{j+k} \frac{\sqrt{l!}}{j!(l-2j)!} \frac{\sqrt{r!}}{k!(r-2k)!} \cdot \\
&\cdot 2^{\frac{l}{2} + \frac{r}{2} - 2j - 2k - 1} \Gamma(\frac{n+l+r-2j-2k+1}{2})],
\end{aligned} \tag{22}$$

where $[\cdot]$ is entier (step) function, Γ is Euler's gamma function. Therefore, the matrix representation of the even power operators \hat{x}^{2p} in the basis \mathcal{B} are hermitean (symmetrical real) matrices with nonzero diagonal and nonzero p subdiagonals (and nonzero p superdiagonals), where the distance of the nearest superdiagonals (or subdiagonals) is 2 (the diagonal is also distant by 2 from the nearest super- and sub-diagonal), whereas the odd power operators \hat{x}^{2p+1} in the basis \mathcal{B} are hermitean (symmetrical real) matrices with zero diagonal and p nonzero subdiagonals (and p nonzero superdiagonals), where the distance of the nearest superdiagonals (or subdiagonals) is 2 (the nearest super- and sub-diagonal are also distant by 2). The physical interpretation of the superdiagonals (and subdiagonals) is connected with the absorption (emission) of phonons.

3 Quantum anharmonic oscillator in $D = 1$ spatial dimension.

Thirdly, we are ready to deal with the quantum anharmonic oscillator in $D = 1$ spatial dimension. Its dimensionless Hamiltonian operator $\hat{\mathcal{H}}_{1,\text{anarm}}^S$ reads:

$$\hat{\mathcal{H}}_{1,\text{anarm}}^S = \hat{\mathcal{H}} + \sum_{s=0}^S a_s \hat{x}^s, \tag{23}$$

where S is a degree of the anharmonicity of the oscillator, and the prefactors a_s are the strengths of anharmonicity. The matrix elements of the anharmonic Hamiltonian operator are:

$$(\hat{\mathcal{H}}_{1,\text{anarm}}^S)_{l,r} = \epsilon_r \delta_{l,r} + \sum_{s=0}^S a_s (\hat{x}^s)_{l,r}, \tag{24}$$

where the representation of the quantum anharmonic oscillator in the quantum harmonic oscillator basis \mathcal{B} is mathematically correct, because the basis \mathcal{B} is a complete set, and the Hilbert space of the eigenfunctions of the anharmonic oscillator is isomorphic to the Hilbert

space \mathcal{V}_1 for the harmonic oscillator, provided that the anharmonic potential:

$$\mathcal{U}_{1,\text{anharmon}}^S(x) = \sum_{s=0}^S a_s x^s, \quad (25)$$

is bounded from below (there are no scattering eigenstates).

Fourthly, we repeat the “Bohigas conjecture” that the fluctuations of the spectra of the quantum systems that correspond classically to the chaotic systems generally obey the spectra of the Gaussian random matrix ensembles. The quantum integrable systems correspond to the classical integrable systems in the semiclassical limit [1, 2]. The probability distributions P_β of the nearest neighbour spacing for the Gaussian orthogonal ensemble GOE(2) of 2×2 Gaussian distributed real-valued symmetric random matrix variables ($\beta = 1$), for the Gaussian unitary ensemble GUE(2) of 2×2 Gaussian distributed complex-valued hermitean random matrix variables ($\beta = 2$), for the Gaussian symplectic ensemble GSE(2) of 2×2 Gaussian distributed quaternion-valued selfdual hermitean random matrix variables ($\beta = 4$), and for the Poisson ensemble (PE) of the random diagonal matrices with homogeneously distributed eigenvalues on the real axis \mathbf{R} are given by the formulae:

$$P_\beta(s) = \theta(s) A_\beta s^\beta \exp(-B_\beta s^2), \quad (26)$$

for the Gaussian ensembles, and

$$P_0(s) = \theta(s) \exp(-s), \quad (27)$$

for the Poisson ensemble, where θ is Heaviside’s unit step function [3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. The constant numbers:

$$A_\beta = 2 \frac{\Gamma^{\beta+1}((\beta+2)/2)}{\Gamma^{\beta+2}((\beta+1)/2)} \quad \text{and} \quad B_\beta = \frac{\Gamma^2((\beta+2)/2)}{\Gamma^2((\beta+1)/2)} \quad (28)$$

are given by the formulae: $A_1 = \pi/2$, $B_1 = \pi/4$ (GOE), $A_2 = 32/\pi^2$, $B_2 = 4/\pi$ (GUE), and $A_4 = 262144/729\pi^3$, $B_4 = 64/9\pi$ (GSE), respectively. For the Gaussian ensembles the energies are characterized by the “level repulsion” of degree β near the origin (vanishing spacing $s = 0$), and the probability distributions P_β vanish at the origin, and the quantum system with “level repulsion” is cast to the class of quantum chaotic systems. For the Poisson ensembles the energies are characterized by the “level clustering” near the origin (vanishing spacing $s = 0$), and the probability distributions P_0 has maximum at the origin, and the quantum system with “level clustering” are treated as the quantum integrable system. After many numerical experiments conducted with different quantum anharmonic oscillators (up to the sextic quantum anharmonic oscillator $S = 6$) we draw conclusion that majority of them behaves like quantum chaotic system, the eigenenergies tend to cluster, the histogram of nearest neighbour spacing is closer to the P_0 distribution resulting from the Poisson ensemble.

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